Hofstadter butterfly and integer quantum Hall effect in three dimensions

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For a three-dimensional lattice in magnetic fields we have shown that the hopping along the third direction, which normally tends to smear out the Landau quantization gaps, can rather give rise to a fractal energy spectram akin to Hofstadter's butterfly when a criterion, found here by mapping the problem to two dimensions, is fulfilled by anisotropic (quasi-one-dimensional) systems. In 3D the angle of the magnetic field plays the role of the field intensity in 2D, so that the butterfly can occur in much smaller fields. The mapping also enables us to calculate the Hall conductivity, in terms of the topological invariant in the Kohmoto-Halperin-Wu's formula, where each of σ_{xy}, σ_{zx} is found to be quantized.

Among the effects of magnetic fields on electronic states, one of the most bizzare is Hofstadter's butterfly. Namely, when a two-dimensional (2D) periodic system is put into a magnetic field, the gap not only appears between the Landau levels, but a series of gaps appear in a selfsimilar fashion as shown by Hofstadter[1]. The butterfly refers to an energy spectrum against the magnetic flux, ϕ, penetrating a unit cell in units of the flux quantum $\phi_0 = h/e$. Usually the butterfly is conceived to be a phenomenon specific to 2D.

Here we raise a question: can we have something like Hofstadter's butterfly in spite of, or even because of, a three-dimensionality (3D)? This may at first seem quite unlikely, since the usual derivation of the butterfly relies on the two-dimensionality of the system, so that a motion along the third direction (z) should tend to wash out the butterfly gaps as well as Landau level gaps. Several authors have extended Hofstadter's problem to 3D in the last decade[2,3], and subbands are indeed shown to overlap or touch with each other. Here we systematically look for the possibility of butterflies (i.e., recursive and fractal gaps) in 3D.

If we do have a butterfly, then we can proceed to question how the integer quantum Hall effect should look like on the butterfly. If one examines a theoretical reasoning from which the quantization in the Hall conductivity is deduced in the usual quantum Hall system, the essential ingredient is the presence of a gap in the energy spectrum. This was indicated in a gauge argument by Laughlin[4], and elaborated by Thouless, Kohmoto, Nightingale, and den Njis[5] when a periodic potential exists. There the quantized Hall conductivity when the Fermi energy, E_F, lies in a butterfly gap is identified to be a topological invariant characterizing the position of gaps.

For 3D Kohmoto, Halperin, and Wu have shown, following the line of the 2D work, that *if* there is an energy gap in a 3D system, then an integer quantum Hall effect should result as long as E_F lies within a gap[6,7]. Montambaux and Kohmoto have actually calculated the Hall conductivity in a case where a third-direction hopping opens some gaps.[8] If butterflies are realized in 3D, we can move on to the systematics of the quantum Hall numbers.

In the present paper we point out that, first, an analog of Hofstadter's butterfly does indeed exist specific to 3D under certain criterion that is fulfilled by anisotropic (quasi-1D) tight-binding lattices in 3D. In this case the butterfly plot refers to energy versus *angle* of the magnetic field. This is obtained by mapping the 3D system to a 2D system. Remarkablly the mapping dictates that the ratio of the magnetic fluxes penetrating two facets of the unit cell plays the role of the magnetic flux in 2D, so that the field intensity B does not have to be strong to realize the butterfly.

More importantly the mapping enables us to systematically calculate the Hall conductivity for the 3D butterfly via identifying the topological invariant in the Kohmoto-Halperin-Wu's formula. We have found that *each of* σ_{xy}, σ_{zx} *is quantized* in 3D.

Our model is non-interacting tight-binding electrons in a uniform magnetic field $\boldsymbol{B}$ described by the Hamiltonian,

$$\mathcal{H} = \sum_{\langle i,j \rangle} (t_{ij} e^{i\theta_{ij}} c_i^\dagger c_j + \text{h.c.}), \tag{1}$$

in standard notations, where the summation is taken over nearest-neighbor sites with $t_{ij} = t_x, t_y, t_z$ along x, y, z, respectively, $\theta_{ij} = (e/\hbar)\int_i^j \boldsymbol{A} \cdot d\boldsymbol{l}$ is the Peierls phase. We first recapitulate the 2D case, because a key in this work is a correspondence between 2D and 3D. In 2D with the Landau gauge $\boldsymbol{A} = (0, Bx)$, y is a cyclic coordinate, so that the wave function becomes $\psi_{lm} = e^{i\nu_y m} F_l$, where (l, m) labels (x, y) coordinates, and ν_y is the Bloch wave

number along y. The Schrödinger equation then takes a form of Harper's equation,

$$-t_x(F_{l-1}+F_{l+1})-2t_y\cos(2\pi\phi l+\nu_y)F_l=EF_l, \quad (2)$$

where $\phi=Bab/\phi_0$ is the number of flux quanta penetrating a unit cell $=a\times b$. While the energy spectrum becomes a butterfly for the ordinary isotropic case, $t_x=t_y$, the gaps are rapidly smeared out as the anisotropy is introduced, $t_y/t_x\to 0$, since the potential term (the cosine function above) weakens. Since t_x and t_y appear on an equal footing, the condition for the appearance of the butterfly in 2D is $t_x\approx t_y$.

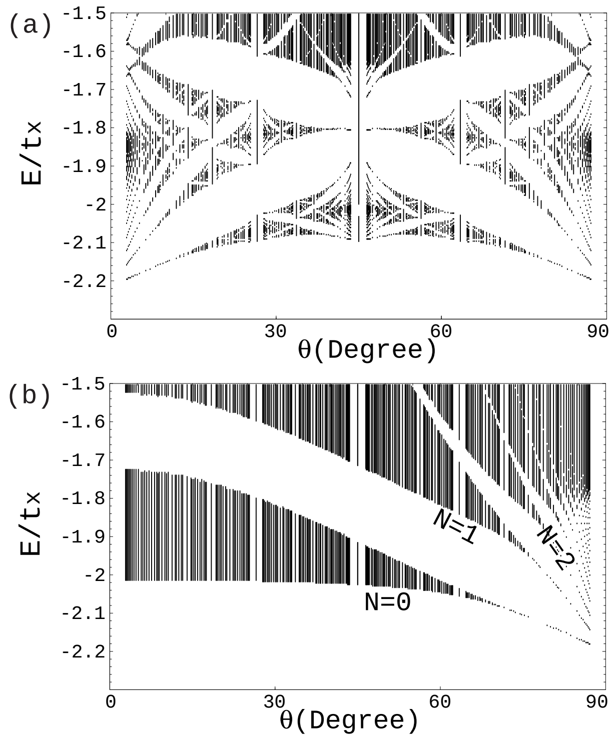

FIG. 1. The energy spectrum of a 3D system with $t_x:t_y:t_z=1:0.1:0.1$ (a) or a 2D system with $t_x:t_y:t_z=1:0.1:0$ (b) plotted against the angle θ in a magnetic field $(\phi_y,\phi_z)=0.2(\sin\theta,\cos\theta)$.

Harper's equation in 3D can be derived in a similar way. For simplicity we consider a simple cubic lattice in a magnetic field $\boldsymbol{B}=(0,B\sin\theta,B\cos\theta)$ assumed to lie in the yz plane. The vector potential is then $\boldsymbol{A}=(0,Bx\cos\theta,-Bx\sin\theta)$, so that y,z are cyclic and the wave function becomes $\psi_{lmn}=e^{i\nu_y m+i\nu_z n}F_l$, where (l,m,n) labels (x,y,z). The Schrödinger equation is

$$\begin{aligned}-t_x(F_{l-1}+F_{l+1})-[2t_y\cos(2\pi\phi_z l+\nu_y)\\ +2t_z\cos(-2\pi\phi_y l+\nu_z)]F_l=EF_l,\end{aligned} \quad (3)$$

where two periodic potentials are now superposed. Here $\phi_y(\phi_z)$ is the number of flux quanta penetrating the side of a unit cell ($=a\times b\times c$) normal to $y(z)$ (inset of Fig.3(a)).

Although the spectrum in 3D does not in general have many gaps (aside from the trivial Bragg-reflection gaps), we first notice that a butterfly-like structure does emerge for certain choices of (t_x,t_y,t_z), as typically displayed in 1(a) for $(t_x,t_y,t_z)=(1,0.1,0.1)$, a quasi-1D system. The spectrum is plotted against the angle θ of a magnetic field $(\phi_y,\phi_z)=0.2(\sin\theta,\cos\theta)$ with $b=c$ assumed here. A structure akin to the 2D butterfly is seen in the bottom (or at the top) of the whole spectrum. One might consider this as a 2D butterfly surviving the third-direction hopping, but this is wrong as is evident from Fig.1(b), where we turn off t_z to find that the spectrum coalesces to a series of broadened Landau levels. So we are talking about the butterfly *specific* to 3D rather than a remnant of a 2D butterfly.

We first explore the mechanism why the butterfly appears in 3D. The doubly periodic potential in the 3D Harper equation comprises $V^{(1)}(l)\propto t_y\cos(2\pi\phi_z l+\nu_y), V^{(2)}(l)\propto t_z\cos(-2\pi\phi_y l+\nu_z)$. We assume that their periods, $1/\phi_z$ and $1/\phi_y$, are much greater than the lattice constant ($\phi_z,\phi_y\ll 1$). We also assume that

$$t_y\phi_z\gg t_z\phi_y, \quad (4)$$

which amounts to an assumption that the local peaks and dips of the total potential $V^{(1)}+V^{(2)}$ is primarily that of $V^{(1)}$.

One can then regard the potential minima of $V^{(1)}$ as 'sites', which we call 'wells' to distinguish from the original sites. The wells are separated by $1/\phi_z$ and feel the slowly-varying $V^{(2)}$. Since each well contains many original sites due to the first assumption, we can talk about bound states for the well in the effective-mass approach. If wells are deep enough, several bound states appear and each state forms a tight-binding band (i.e., Landau band), and the equation (3) reduces to

$$\begin{aligned}-t'(J_{l'-1}+J_{l'+1})-2t_z\cos[-2\pi(\phi_y/\phi_z)l'\\ +(\phi_y/\phi_z)\nu_y+\nu_z]J_{l'}=EJ_{l'}.\end{aligned} \quad (5)$$

Here t' is a transfer integral between neighboring wells labelled by l', $J_{l'}$ the 'effective-mass' wave function, and the cosine term is the value of $V^{(2)}$ at each minimum of $V^{(1)}$. The reduced equation has exactly the same form as that of the 2D system, eqn.(2) if we translate

$$3\text{D}:(t_x,t_y,t_z,\phi_y,\phi_z)\longrightarrow 2\text{D}:(t',t_z,\phi_y/\phi_z). \quad (6)$$

Since the butterfly is a hallmark of an isotropic 2D case, one can predict that the subband in 3D for which $t'\approx t_z$ should exhibit a butterfly.

We can estimate t' by applying the effective-mass approximation to Harper's equation (3). We first convert the equation (when there is $V^{(1)}$ alone) to a differential equation for a continuous variable $\tilde{l}\equiv 2\pi\phi_z l$, which turns out to contain a combination t_y/ϕ_z^2 only (with $t_x=1$, a unit of energy). Since t' is a matrix element of $V^{(1)}\propto t_y$, we have a simple scaling law,

$$t' = 2t_y \ f\left(\frac{t_y}{\phi_z^2}\right). \qquad (7)$$

Note that the value of t' differs from one tight-binding band to another, where middle bands, with weaker binding, have larger t'.

We have then numerically calculated $t'(t_y, \phi_z)$ for the lowest band. With the scaling, the t_y-dependence of t' for a particular ϕ_z provides the whole dependence, shown in Fig.2. If we plug in the condition for the butterfly, $t_z \simeq t'$, the plot indicates how to adjust ϕ_z to have a butterfly for given (t_y, t_z). One can immediately find that the butterfly is restricted to the case with $t_y, t_z \ll 1(= t_x)$, i.e., quasi-1D systems. This is because ϕ_z becomes too large to satisfy $\phi_z \ll 1$ in the most region of $t_y \approx 1$ or in the region $t_z \approx 1$ (out of the plot).

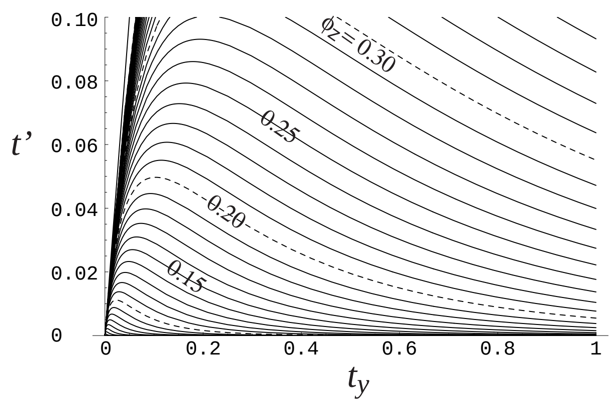

FIG. 2. The effective transfer $t'(t_y, \phi_z)$ for the lowest Landau band in units where $t_x = 1$. By plugging $t' \simeq t_z$, the plot serves to identify appropriate values of ϕ_z to realize the butterfly for given (t_y, t_z).

This plot shows that the above example, $(t_x, t_y, t_z) = (1, 0.1, 0.1)$, is indeed a right choice, for which we can show that $t' = 0.05 \approx t_z(= 0.1)$ for the lowest subband. Incidentally, the butterfly is symmetric in this example, which is an accident for $t_y = t_z$: in Harper's equation $V^{(1)}$ and $V^{(2)}$ exchange roles at $\theta = 45°$ for $t_y = t_z$. Around 45°, or more generally around $t_y\phi_z \approx t_z\phi_y$, the above argument breaks down but a clear structure remains. We can explain this as follows. When $t_y\phi_z \approx t_z\phi_y$, $V^{(1)}+V^{(2)}$ exhibits a beat so that the barrier height separating the wells varies from place to place, which implies that t' varies from place to place. However, a change in the wall height (t_y) changes t' only slightly, since t' has a broad peak in Fig.2.

Thus in 3D the effective flux in eqn.(6) is a ratio ϕ_y/ϕ_z. In 2D by contrast, a butterfly requires $\phi \sim O(1)$, i.e., B has to be impossibly large ($\sim 10^5$T for $a = 2$Å). Would this render the 3D butterfly experimentally feasible?[9] In principle, Fig.2 shows that there exists appropriate (t_y, t_z) no matter how small ϕ_z may be. In practice, (t_y, t_z) become smaller as ϕ_z decreases, and the energy scale (width of the Landau band $4(t' + t_z)$ with $t' \approx t_z$) shrinks for smaller ϕ_z, so that it will be hard to resolve the butterfly structure. For typical quasi-1D organic conductors such as $(TMTSF)_2X$ we have $t_x : t_y : t_z = 1 : 0.1 : 0.01$ with $a, b, c \sim 10$Å, and we can estimate the required $\phi_z \sim 0.1$, which corresponds to $B \sim 400$T. It is still huge, but much smaller than the value required for 2D and around the border of experimental feasibility.[10]

While we have discussed appropriate values for given (t_y, t_z), are there restrictions on (t_y, t_z) to have butterflies? Binding of a well must be so strong that the transfer to second neighbors is negligible. If one approximates a well in $V^{(1)}$ with a harmonic potential, the quantized energies are $(n + \frac{1}{2})\hbar\omega$. Then the n-th state is strongly bound to each well when this energy is smaller than $4t_y$, the depth of a well. Hence t_y should not be too small $(\sqrt{t_y} > \phi_z)$, otherwise we have trivial Bragg-reflection gaps only. Also, the residual potential $V^{(2)}$ whose amplitude is $2t_z$ must be weaker than $\hbar\omega$ (i.e., $t_z < \phi_z\sqrt{t_y}$) so that different Landau bands are not mixed. All the conditions (those discussed in this paragraph as well as $\phi_z, \phi_y \ll 1, t_y\phi_z \gg t_z\phi_y$) can be interpreted in the semiclassical quantization involving the cross sections of equipotential surfaces, but the essential hopping (t') between adjacent cross-sectional orbits is outside the scope of the semiclassical picture.

Now we come to our goal of calculating the Hall conductivity when the Fermi level lies in each gap of the 3D butterfly. The mapping does indeed enables us to accomplish this through identifying the topological invariants in the general formula for the Hall conductivity for 3D Bloch electrons by Kohmoto-Halperin-Wu. In the formula the Hall conductivity tensor is expressed as

$$\sigma_{ij} = -\frac{e^2}{2\pi h}\sum_k \epsilon_{ijk} G_k \qquad (8)$$

when Fermi energy is in a gap. Here ϵ_{ijk} is a unit antisymmetric tensor, $\boldsymbol{G} = \mu_1\boldsymbol{a}^* + \mu_2\boldsymbol{b}^* + \mu_3\boldsymbol{c}^*$ with $\boldsymbol{a}^*, \boldsymbol{b}^*, \boldsymbol{c}^*$ being the primitive reciprocal lattice vectors, and μ_1, μ_2, μ_3 are topological invariants specifying each gap (i.e., remain constant when we change the direction of B in the present context). For an orthogonal lattice we have simply $\sigma_{yz} = -\frac{e^2}{h}\frac{\mu_1}{a}$, $\sigma_{zx} = -\frac{e^2}{h}\frac{\mu_2}{b}$, $\sigma_{xy} = -\frac{e^2}{h}\frac{\mu_3}{c}$.

So we have only to determine invariant integers, which are subject to a Diophantine equation,

$$\frac{r}{Q} = \lambda + \frac{P}{Q}n_x\mu_1 + \frac{P}{Q}n_y\mu_2 + \frac{P}{Q}n_z\mu_3, \qquad (9)$$

where we have assumed a rational magnetic flux, $(\phi_x, \phi_y, \phi_z) = \frac{P}{Q}(n_x, n_y, n_z)$ (P, Q: integers, n_x etc have no common divisors), r the number of occupied bands, and λ another topological invariant. Although the solution of the Diophantine equation is not unique, Thouless *et al.*[5] argued for 2D that there is a restriction on the integers that decides the solution uniquely. Kohmoto *et al.*[7] conjecture the uniqueness of the solution in 3D in analogy with the 2D case, where the restriction for 3D reads $|\mu_1 n_x + \mu_2 n_y + \mu_3 n_z| < Q/2$.

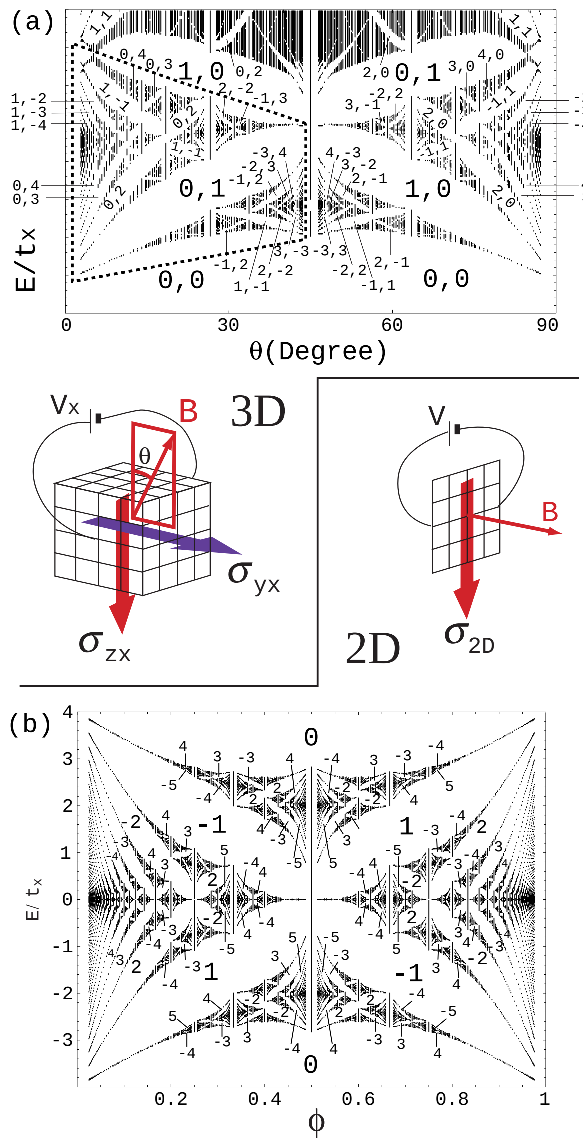

FIG. 3. (a) The conductivity $(\sigma_{xy}, \sigma_{zx}) = -e^2/h(\mu_3, \mu_2)$ is plotted on a 3D butterfly, where we display the topological invariants (μ_3, μ_2) for each gap. (b) The corresponding plot for $\sigma_{2D} = -(e^2/h)t$ on the 2D butterfly. The area enclosed by a dashed line in (a) corresponds to the 2D butterfly. μ_2 in (a) corresponds to t in (b), while μ_3 in (a) to s in Eq.(10)

We can then calculate the Hall conductivity for the 3D butterfly. We assume $(\phi_x, \phi_y, \phi_z) = P/Q(0, n_y, n_z)$ and $t_y\phi_z \gg t_z\phi_y$, for which the effective flux in eq.(5) is $\phi = \phi_y/\phi_z = n_y/n_z$. Hence each Landau band should split into n_z butterfly subbands. Let us consider the situation where E_F lies just above the mth subband in the lth Landau band from the bottom, i.e., $(ln_z + m)$ subbands altogether. Each subband is shown to comprise P bands, so that the gap has an index $r = (ln_z + m)P$. Substituting this in the Diophantine eq.(9), we have $(ln_z + m)P = Q\lambda + Pn_y\mu_2 + Pn_z\mu_3$. Since P and Q have no common divisors, s must be a multiple of P, and with the above restriction one has $\lambda = 0$, and we end up with $ln_z + m = n_y\mu_2 + n_z\mu_3$ for the 3D butterfly in the lower half of the entire band. Thus we can determine μ_2, μ_3 for an arbitrary gap in the 3D butterfly as explicitly displayed in Fig.3(a).

If we compare with a corresponding plot for 2D in Figure 3(b), we recognize a beautiful consequence of the 2D-3D mapping established here as a unsuspected one-to-one correspondence between the Hall conductivities on 2D and 3D butterflies *as a whole* (i.e., for a set of topological invariants attached to the recursive gaps). Namely, the Hall conductivity in 2D[5] is given by $\sigma_{\rm 2D} = -\frac{e^2}{h}t$, where t is an integer in a 2D Diophantine equation $r = qs + pt$. If we compare this with the 3D Diophantine equation, $m = n_z(\mu_3 - l) + n_y\mu_2$, the mapping dictates a correspondence $n_y \leftrightarrow p$, $n_z \leftrightarrow q$, $m \leftrightarrow r$, so that the invariant integers should translate as

$$\mu_3 - l \longleftrightarrow s, \; \mu_2 \longleftrightarrow t. \qquad (10)$$

This implies that σ_{zx} in 3D plays the role of $\sigma_{\rm 2D}$.

Future problems are to extend the effective theory to the the arbitrary orientation of $\boldsymbol{B}$, for which Harper's equation in the arbitrary $\boldsymbol{B}$ has been discussed in an existing literature[2,3]. We wish to thank Mahito Kohmoto for discussions.

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